

Fermi excitations in a trapped atomic Fermi gas with a molecular Bose condensate

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(Dated: February 2, 2008)

We discuss the effect of a molecular Bose condensate on the energy of Fermi excitations in a trapped two-component atomic Fermi gas. The single-particle Green's functions can be approximated by the well-known BCS form, in both the BCS (Cooper pairs) and BEC (Feshbach resonance molecules) domains. The composite Bose order parameter $\tilde{\Delta}$ describing bound states of two atoms and the Fermi chemical potential μ are calculated self-consistently. In the BEC regime characterized by $\mu < 0$, the Fermi quasiparticle energy gap is given by $\sqrt{\mu^2 + \tilde{\Delta}^2}$, instead of $|\tilde{\Delta}|$ in the BCS region, where $\mu > 0$. This shows up in the characteristic energy of atoms from dissociated molecules.

PACS numbers: 03.75.Ss, 05.30.Jp, 74.20.Mn

There has been increasing interest in the BCS-BEC crossover in a two-component trapped atomic Fermi gas[1, 2, 3]. This recent theoretical work has extended the classic work in superconductors[4, 5, 6, 7] to include a Feshbach resonance[8, 9]. This allows one to both increase the attractive interaction[8, 9] by working above the resonance as well as to include the effect of long-lived dimer molecules just below the resonance. Several groups[10, 11, 12] have presented evidence for a molecular Bose condensate in a two-component Fermi gas in the region $a_s^{2b} > 0$, where a_s^{2b} is the two-body s -wave scattering length. Recent theories[1, 2, 3] clearly show that a unified description of both the BEC and BCS limits can be given, in terms of a *composite* order parameter which involves a Cooper pair condensate and a molecular Bose condensate associated with the Feshbach resonance. They are two limits of a superfluid Fermi gas, both arising from a Bose condensate of bound states. The only difference lies in the origin of these bound states.

This similarity has been noted in the study of the collective modes of this condensate in the BCS and BEC limits[13, 14] as well as in the crossover region[2]. In the present letter, we emphasize this similarity by considering the single-particle Fermi quasiparticle spectrum in the BCS-BEC crossover region with a Feshbach resonance. We point out that the well-known BCS-Bogoliubov excitation spectrum is a good approximation in both the BCS and BEC limits[2] at all temperatures in the superfluid phase. In particular, the Fermi excitations exhibit an energy gap due to their coupling to a molecular Bose condensate, the analogue of what happens in the classic BCS limit. Our work emphasizes the importance of measuring[15] the energy and momentum of single-particle excitations in trapped superfluid Fermi gases as a way of studying the effect of the molecular Bose condensate. We do not address possible corrections very close to the Feshbach resonance in the unitarity limit ($k_F a_s^{2b} \rightarrow \pm\infty$).

We consider a gas of Fermi atoms composed of two atomic hyperfine states (labeled by $\sigma = \uparrow, \downarrow$), coupled

to a molecular two-particle bound state. The coupled fermion-boson model Hamiltonian is given by[1, 8, 9, 16]

$$\begin{aligned} \hat{H} = & \sum_{\mathbf{p}\sigma} \varepsilon_{\mathbf{p}} c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} + \sum_{\mathbf{q}} (\varepsilon_{B\mathbf{q}} + 2\nu) b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \\ & - U \sum_{\mathbf{p}, \mathbf{p}', \mathbf{q}} c_{\mathbf{p}+\mathbf{q}/2\uparrow}^\dagger c_{-\mathbf{p}+\mathbf{q}/2\downarrow}^\dagger c_{-\mathbf{p}'+\mathbf{q}/2\downarrow} c_{\mathbf{p}'+\mathbf{q}/2\uparrow} \\ & + g_r \sum_{\mathbf{p}, \mathbf{q}} [b_{\mathbf{q}}^\dagger c_{-\mathbf{p}+\mathbf{q}/2\downarrow} c_{\mathbf{p}+\mathbf{q}/2\uparrow} + \text{h.c.}] \end{aligned} \quad (1)$$

For simplicity, we discuss the case of a *uniform* two-component Fermi gas, although results in the figures take into account an isotropic harmonic trap potential. In Eq. (1), a Fermi atom and a Boson associated with the Feshbach resonance are, respectively, described by the destruction operators $c_{\mathbf{p}\sigma}$ and $b_{\mathbf{q}}$. The kinetic energy of a bare Fermi atom is $\varepsilon_{\mathbf{p}} \equiv p^2/2m$ and $\varepsilon_{B\mathbf{q}} + 2\nu \equiv q^2/2M + 2\nu$ is the excitation spectrum of the bare b -molecular bosons. The lowest energy of the b -bosons (2ν) is the threshold energy of the Feshbach resonance. The last term in Eq. (1) is the Feshbach resonance with a coupling constant g_r , which describes how a b -molecule can dissociate into two Fermi atoms and how two Fermi atoms can form one b -boson. Eq. (1) also includes the usual attractive interaction $-U$ (< 0) arising from nonresonant processes.

Since a b -Bose molecule consists of a bound state of two Fermi atoms, the boson mass is $M = 2m$ and the conservation of the total number of particles N imposes the relation

$$N = \sum_{\mathbf{p}\sigma} \langle c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} \rangle + 2 \sum_{\mathbf{q}} \langle b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \rangle. \quad (2)$$

We incorporate this crucial constraint into the model Hamiltonian in Eq. (1) using a single chemical potential and work with $\mathcal{H} \equiv H - \mu N$. This leads to a shift in the energies, $\varepsilon_{\mathbf{p}} \rightarrow \xi_{\mathbf{p}} \equiv \varepsilon_{\mathbf{p}} - \mu$ and $\varepsilon_{B\mathbf{q}} + 2\nu \rightarrow \xi_{B\mathbf{q}} \equiv \varepsilon_{B\mathbf{q}} + 2\nu - 2\mu$.

The mean-field approximation (MFA) for the coupled Fermi-Bose Hamiltonian reduces to[16, 17]

$$\begin{aligned}\mathcal{H}_{\text{MFA}} = & \sum_{\mathbf{p}\sigma} \xi_{\mathbf{p}} c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} - \sum_{\mathbf{p}} [\Delta c_{\mathbf{p}\downarrow} c_{-\mathbf{p}\uparrow} + h.c.] \\ & + \sum_{\mathbf{q}\neq 0} \xi_{B\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + g_r \sum_{\mathbf{p}} [\phi_m c_{\mathbf{p}\downarrow} c_{-\mathbf{p}\uparrow} + h.c.],\end{aligned}\quad (3)$$

where the Cooper pair order parameter is $\Delta \equiv U \sum_{\mathbf{p}} \langle c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow} \rangle$ and the molecular condensate is described by $\phi_m \equiv \langle b_{\mathbf{q}=0} \rangle$. Thus the MFA broken symmetry state is described by

$$\begin{aligned}\mathcal{H}_{\text{MFA}} = & \sum_{\mathbf{p}\sigma} \xi_{\mathbf{p}} c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} + \sum_{\mathbf{q}\neq 0} \xi_{B\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \\ & - \sum_{\mathbf{p}} [\tilde{\Delta} c_{\mathbf{p}\downarrow} c_{-\mathbf{p}\uparrow} + h.c.],\end{aligned}\quad (4)$$

where the composite order parameter is given by $\tilde{\Delta} = \Delta - g_r \phi_m$. The molecular Bose condensate ϕ_m and the Cooper pair order parameter Δ are strongly hybridized. One can also show that[1, 2, 3, 8, 9]

$$\phi_m = -\frac{g_r}{2\nu - 2\mu} \left(\frac{\Delta}{U} \right), \quad (5)$$

which leads to a renormalized pairing interaction U_{eff}

$$\tilde{\Delta} = U_{\text{eff}} \sum_{\mathbf{p}} \langle c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow} \rangle, \quad U_{\text{eff}} = U + \frac{g_r^2}{2\nu - 2\mu}. \quad (6)$$

In recent discussions on the BCS-BEC crossover (for example, Refs. [18, 19]), the Feshbach resonance is often only included to the extent that the order parameter $\tilde{\Delta}$ in Eq. (6) involves the correct two-body *s*-wave scattering length given by $-4\pi a_s^{2b} \hbar^2/m = U + g_r^2/2\nu$. The two-body Feshbach resonance at $2\nu = 0$ occurs at the resonance value B_0 of the magnetic field. Such calculations are identical to the original theories of the BCS-BEC crossover in superconductors[4, 6, 7]. No explicit account is taken of the formation of a *b*-molecule condensate described by ϕ_m , as done in the above MFA calculation, which leads to the effective pairing interaction in Eq. (6)[1, 2, 3].

Using the simple pairing MFA summarized by Eqs. (4)-(6) gives the usual BCS-Gor'kov expressions for the diagonal and off-diagonal single-particle Green's functions

$$G_{11}(\mathbf{p}, \omega) = \frac{\omega + \xi_{\mathbf{p}}}{\omega^2 - E_{\mathbf{p}}^2}, \quad G_{12}(\mathbf{p}, \omega) = -\frac{\tilde{\Delta}}{\omega^2 - E_{\mathbf{p}}^2}, \quad (7)$$

with the BCS-Bogoliubov excitation energy given by

$$E_{\mathbf{p}} = \sqrt{(\varepsilon_{\mathbf{p}} - \mu)^2 + |\tilde{\Delta}|^2}. \quad (8)$$

Using $G_{12}(\mathbf{p}, \omega)$ to calculate Δ , one finds that $\tilde{\Delta}$ satisfies the “gap equation” with the pairing interaction U_{eff} ,

$$\tilde{\Delta} = U_{\text{eff}} \sum_{\mathbf{p}} \frac{\tilde{\Delta}}{2E_{\mathbf{p}}} \tanh \frac{1}{2} \beta E_{\mathbf{p}}. \quad (9)$$

As usual, a cutoff is introduced in the momentum summation[1, 3]. At this MFA level, the total number of atoms at $T = 0$ is

$$N = N_F + 2N_B^c, \quad (10)$$

where the number of Fermi atoms is given [using $G_{11}(\mathbf{p}, \omega)$] by the well-known expression

$$N_F = \sum_{\mathbf{p}, \sigma} \langle c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} \rangle = \sum_{\mathbf{p}} \left[1 - \frac{\xi_{\mathbf{p}}}{E_{\mathbf{p}}} \tanh \frac{1}{2} \beta E_{\mathbf{p}} \right]. \quad (11)$$

The number of Bose-condensed *b*-molecules is $N_B^c = |\phi_m|^2$, where ϕ_m is determined by $\tilde{\Delta}$ and μ .

We briefly sketch how one proceeds in the case of an isotropic harmonic trap[20]. We expand the fermion quantum field operator $\hat{\Psi}_\sigma(\mathbf{r})$ and boson operator $\hat{\Phi}(\mathbf{r})$ in terms of the single-particle eigenfunctions $f_{nlm}(\mathbf{r}) \equiv u_{nl}(r)Y_{lm}(\theta, \phi)$ of the harmonic potential, with energy $\xi_{nl} = (2n + l + 3/2)\hbar\omega_0$. The resulting MFA Hamiltonian, which corresponds to Eq. (4) for a uniform gas, is given by[21]

$$\begin{aligned}\mathcal{H}_{\text{MFA}} = & \sum_{nlm, \sigma} \xi_{nl} c_{nlm\sigma}^\dagger c_{nlm\sigma} + \sum_{nlm} \xi_{nl}^B b_{nlm}^\dagger b_{nlm} \\ & - \sum_{nn'l'm} F_{nn'}^l [c_{nlm\uparrow}^\dagger c_{n'l-m\downarrow}^\dagger + h.c.].\end{aligned}\quad (12)$$

Here c_{nlm}^\dagger (b_{nlm}) is the creation operator of an atom (molecule) in the state $f_{nlm}(\mathbf{r})$ ($f_{nlm}^B(\mathbf{r})$). $F_{nn'}^l$ arises from the pair potential, $F_{nn'}^l \equiv \int_0^\infty r^2 dr \Delta(r) u_{nl}(r) u_{n'l'}(r)$. Eq. (12) can be diagonalized by the usual BCS-Bogoliubov transformation. One can calculate $\Delta(r) = U \langle \hat{\Psi}_\downarrow(\mathbf{r}) \hat{\Psi}_\uparrow(\mathbf{r}) \rangle$ as well as N_F in Eq. (10), by expanding the fermion operators in terms of the BCS-Bogoliubov excitation operators. Using the generalization of Eq. (5),

$$\frac{g_r}{U} \Delta(r) + \left(-\frac{\hbar^2 \nabla^2}{2M} + \frac{1}{2} M \omega_0^2 r^2 + 2\nu - 2\mu \right) \phi_m(r) = 0, \quad (13)$$

we can determine $\phi_m(r)$ from $\Delta(r)$, and hence find the composite order parameter $\tilde{\Delta}(r)$ in $F_{nn'}^l$, as well as N_B^c .

The values of μ and $\tilde{\Delta}$ are determined by the self-consistent solutions of the MFA gap equation (9) and the number equation given by Eqs. (10) and (11). This simple “pairing approximation” for the single-particle excitations is expected to give a quantitative description at $T = 0$ (where $\tanh \frac{1}{2} \beta E_{\mathbf{p}} \rightarrow 1$) since fluctuations are small and all the *b*-molecules are Bose-condensed. This $T = 0$ limit was first studied by Leggett[4] in the absence of a Feshbach resonance. For T approaching T_c , however, the fluctuations associated with exciting *b*-molecules out of the condensate and coupling to the particle-particle (Cooper-pair) channel become increasingly important[1, 3]. These fluctuations (rather than the breaking up of two-particle bound states) determine T_c and the region above, as first discussed by Nozières and

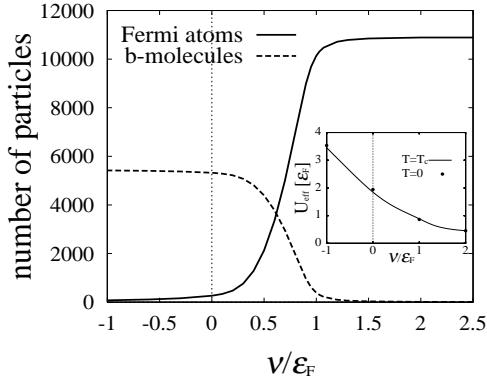


FIG. 1: The number of particles as a function of the threshold energy 2ν in a trapped superfluid Fermi gas at $T = 0$. The Fermi energy $\varepsilon_F = 31.5\hbar\omega_0$ is for a free gas with $N = 10912$ atoms. Figs. 1-3 are for $U = 0.52\varepsilon_F$ and $g_r = 0.2\varepsilon_F$. The inset shows U_{eff} in a *uniform* Fermi gas, for $U = 0.3\varepsilon_F$ and $g_r = 0.6\varepsilon_F$. μ is almost temperature independent below T_c , as is U_{eff} .

Schmitt-Rink (NSR)[5]. Ref. [1] generalized the NSR approach to deal with a Feshbach resonance by including the contribution of *b*-molecules *outside* the condensate (ignored in Eq. (10)) in determining μ at T_c .

In Ref. [2], we extended the NSR approach to discuss the superfluid phase *below* T_c in a uniform Fermi gas. Both $\tilde{\Delta}$ and μ are obtained by solving Eqs. (9) and (10) self-consistently, but now including the depletion of $\tilde{\Delta}$ through the presence of non-Bose-condensed *b*-molecules[22]. This procedure gives the simplest “renormalization” of the MFA-BCS single-particle results in Eqs. (7) and (8), which now involve values of μ and $\tilde{\Delta}$ which include the effect of fluctuations around the MFA theory. The physics of this is most clearly shown in a functional integral treatment[23]. The gap equation (9) determines the MFA saddle point minimum, while the new number equation (10) describes the effect of Gaussian fluctuations around the MFA saddle point. The latter gives rise to a renormalized value of the chemical potential μ occurring in the MFA gap equation, which in turn leads to a renormalized value of $\tilde{\Delta}$. It is important to note that this renormalized pairing approximation generates response functions[2] which exhibit gapless Goldstone modes, a crucial requirement of a conserving many-body approximation. Here we use the $T = 0$ results to illustrate the behavior in a trapped Fermi gas[20].

In Fig. 1, we illustrate how N_F and N_B vary as a function of the *b*-molecule threshold 2ν for a trapped Fermi gas at $T = 0$ [20]. The molecular condensate region [10, 11, 12] occurs just below the two-body Feshbach resonance at $2\nu = 0$, where a_s^{2b} is large and positive, leading to stable (long-lived) *b*-molecules. In Fig. 1, the Fermi contribution includes the Cooper pairs. The latter contribution becomes less important for $2\nu < 2\varepsilon_F$ and is almost absent relative to the *b*-molecules as soon as one passes through the Feshbach resonance (when $\nu < 0$, one has $a_s^{2b} > 0$). A more detailed decomposition into Fermi

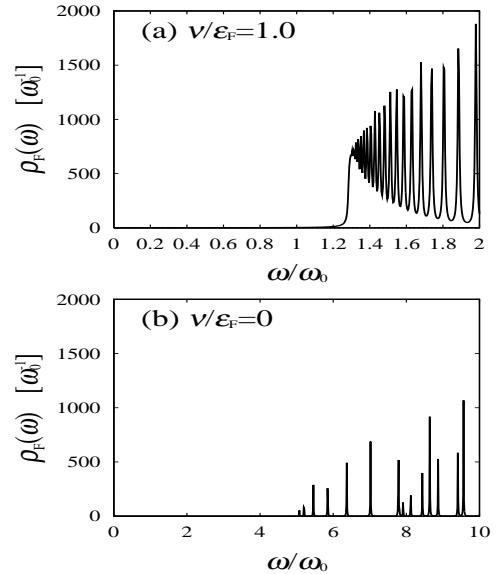


FIG. 2: Single-particle spectral density in a trapped gas of Fermi atoms at $T = 0$. The sharp peaks reflect the discrete BCS-Bogoliubov energies in a harmonic potential.

excitations, Cooper-pairs and *b*-molecules is given at T_c in Ref. [1], which may be more relevant to the region just below T_c studied in Refs. [10, 11, 12].

In our pairing approximation, the effective attractive interaction U_{eff} in Eq. (6) plays a crucial role. One finds that U_{eff} smoothly increases in magnitude as ν decreases, with nothing unusual happening at the two-body Feshbach resonance at $2\nu = 0$ (see the inset in Fig. 1).

As discussed in Ref. [2], the BCS-Bogoliubov quasiparticle spectral density is easily calculated from

$$\rho_F(\omega) \equiv -\frac{1}{\pi} \sum_{\mathbf{p}} \text{Im}[G_{11}(\mathbf{p}, \omega + i0^+)]. \quad (14)$$

The spectral density for a uniform gas at $T = 0$ is shown in Fig. 8 in Ref. [2]. In the BEC region $2\nu \lesssim 0$, we have $\mu < 0$ and as a result, $\rho_F(\omega)$ has an excitation energy gap which starts at $\omega = \sqrt{\mu^2 + |\tilde{\Delta}|^2}$ for excitations with $\mathbf{p} = 0$ [4, 7]. In the BCS region $2\nu > 0$ (where $\mu > 0$), the quasiparticle gap starts at $\omega = |\tilde{\Delta}|$, from Fermi quasiparticles with momentum $p = \sqrt{2m\mu}$. In Fig. 2, we compare the density of states $\rho_F(\omega)$ at $\nu = \varepsilon_F$ (BCS) with the result at the Feshbach resonance $\nu = 0$ (BEC) in a trap. The sharp peaks correspond to the BCS-Bogoliubov excitation frequencies obtained from numerically solving[20] the Bogoliubov-de Gennes coupled equations, together with a self-consistent calculation of μ and $\tilde{\Delta}(\mathbf{r})$ as described above. The sharp excitation edge in Fig. 2(a) reflects the BCS density of states (DOS) $\rho_F(\omega) \sim \text{Re}[\frac{\omega}{\sqrt{\omega^2 - |\tilde{\Delta}|^2}}]$, which is absent in the BEC region shown in Fig. 2(b).

The threshold energy of the continuum spectrum in the density response function[2] is equal to the minimum energy needed to break a bound pair of atoms and put

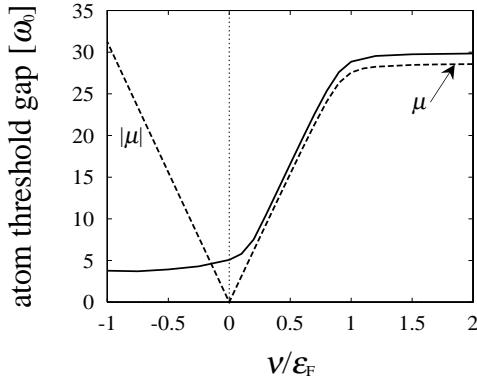


FIG. 3: Energy gap for atoms vs ν in a superfluid Fermi gas at $T = 0$ trapped in a harmonic potential.

them into the lowest energy states. This is the binding energy E_{BE} of the dimer in the interacting Fermi gas. In the JILA experiments[10, 24], a r.f. pulse of energy $h\nu_{\text{r.f.}}$ is used to stimulate a transition to a lower Zeeman state. The two atoms will share an excess energy $\Delta E = h\nu_{\text{atom}} - h\nu_{\text{r.f.}} - E_{\text{BE}}$, where $h\nu_{\text{atom}}$ is the atom-atom transition frequency. If the dissociated pair of atoms are in the \uparrow ($m_F = -9/2$) and \downarrow ($m_F = -7/2$) states involved in the molecular Bose condensate, the energy of each atom (E_{atom}) will have a threshold E_g given by $E_{\text{atom}} \geq E_g = \sqrt{\mu^2 + |\tilde{\Delta}|^2 - |\mu|}$ in the BEC region ($\mu < 0$), with the atoms having very small momentum. For $\tilde{\Delta} \ll |\mu|$, this gap $E_g \simeq |\tilde{\Delta}|^2/2|\mu|$ is very small. The excess energy ΔE will be shared by the dissociated atoms, with $E_{\text{atom}} = E_g + \frac{\Delta E}{2}$. In contrast, one has $E_g = |\tilde{\Delta}| + \mu$ in the BCS region ($\mu > 0$), with the atoms having a large momentum ($p = \sqrt{2m\mu}$) comparable to the Fermi momentum ($\mu \sim \epsilon_F \gg |\tilde{\Delta}|$). In Fig. 3, we plot E_g as a function of ν in a trapped Fermi gas at $T = 0$. Of course, these predictions assume that the dissociated

atoms have thermalized with the rest of the atoms in the Fermi gas, so that the excitation spectrum is described by the equivalent of Eq. (8).

By way of contrast, if the r.f. pulse dissociates the molecule into atoms in the spin state \uparrow ($m_F = -9/2$) and another Zeeman state ($m_F = -5/2$ in Ref. [10]), only the \uparrow atom will be coupled to the underlying molecular condensate involving (\uparrow, \downarrow) -pairs. This atom will exhibit an energy gap E_g associated with the finite value of the order parameter $|\tilde{\Delta}|$. The other atom will not have an energy gap. One sees that the energy of the pair of dissociated atoms can be different, assuming that a molecular condensate is only coupled to one of them. The energy and momentum spectrum of dissociated atoms should be a very direct probe of the presence (or absence) of a Bose condensate (see also Refs.[15, 18] for other techniques to study single-particle excitations).

In summary, we recall that in the original work on the BCS-BEC crossover[4, 5, 6, 7], the only bound states were Cooper pairs, whose existence is a many-body effect and does not require a two-body resonance. In this case, when $a_s > 0$, the Cooper pairs are long-lived and form a molecular condensate. In contrast, in the presence of a Feshbach resonance, the condensate is formed of stable dimer molecules in the BEC limit, with a negligible contribution from Cooper pairs. We have studied the single-particle quasiparticle spectrum associated with a *composite* Bose order parameter arising from the formation of a BEC of Cooper pairs and Feshbach-induced molecules. We have emphasized that a simple static MFA pairing approximation renormalized to include fluctuations[2, 5] describes *both* the BCS limit (where Cooper pairs dominate) and the BEC limit (where stable Feshbach molecules dominate). Both regions are described by a renormalized BCS-type single-particle Fermi spectrum.

Y. O. was supported by a University of Tsukuba Research Project and A. G. by NSERC of Canada.

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